

## Numerical Treatment of ODE

- remember population dynamics: one or some ODE
  - there as an **initial value problem**: starting point given
  - sometimes also as a **boundary value problem**: starting and final point given (think of a space shuttle's trajectory, e.g.)

- prototypes of an initial value problem (IVP):

$$\dot{y}(t) = f(t, y(t)), \quad y(a) = y_a, \quad t \geq a$$

$$\dot{y}_i(t) = f_i(t, y_1(t), \dots, y_n(t)), \quad y_i(a) = y_{i,a}, \quad t \geq a, \quad i = 1, \dots, n$$

- if  $f$  depends on  $t$  only: simple integration or *quadrature*

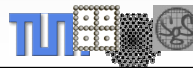
- standard approach for IVP: finite difference approximation (difference quotient instead of derivative)

$$y(a + \delta t) \doteq y(a) + \delta t \cdot f(t, y(a))$$

$$y_{k+1} = y_k + \delta t \cdot f(t_k, y_k), \quad t_k = a + k\delta t, \quad k = 0, 1, \dots$$



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## Euler's Method, Discretization Error

- this is the simplest strategy and called *Euler's method*
- other derivation: truncated Taylor expansion of  $y(t)$

$$y(t_{k+1}) = y(t_k) + (t_{k+1} - t_k) \dot{y}(t_k) + R \doteq y(t_k) + (t_{k+1} - t_k) f(t_k, y_k)$$

- local discretization error: local influence of using differences instead of derivatives; here:

$$l(\delta t) = \max_{[a,b]} \{ |y(t + \delta t) - y(t) - \delta t \cdot f(t, y(t))| \}$$

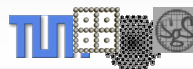
- global discretization error: maximum error of all computed discrete approximations:

$$e(\delta t) = \max_{[a,b]} \{ |y_k - y(t_k)| \}$$

- consistency:  $l(\delta t) \rightarrow 0$  for  $\delta t \rightarrow 0$
- convergence (stronger):  $e(\delta t) \rightarrow 0$  for  $\delta t \rightarrow 0$



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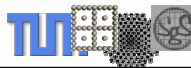
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## Order of Convergence

- Euler (some restrictions with respect to  $y$  and  $f$ ):
  - consistent of *first order*:  $l(\delta t) = O(\delta t)$
  - convergent of *first order*:  $e(\delta t) = O(\delta t)$
  - There are methods that are consistent but do not converge!
- look for higher-order methods (faster convergence)
  - start from Taylor expansion: leads to complicated formulas (higher derivatives of  $f$ ) ☹
  - use additional evaluations of  $f$ : Runge-Kutta-type methods
- simplest representative: method of Heun

$$y_{k+1} = y_k + \frac{\delta t}{2} (f(t_k, y_k) + f(t_{k+1}, y_k + \delta t \cdot f(t_k, y_k)))$$

- both consistent and convergent of second order



## Method of Runge and Kutta

- most famous representative: Runge-Kutta method

$$y_{k+1} = y_k + \frac{\delta t}{6} (T_1 + 2T_2 + 2T_3 + T_4),$$

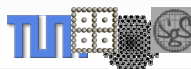
$$T_1 = f(t_k, y_k),$$

$$T_2 = f\left(t_k + \frac{\delta t}{2}, y_k + \frac{\delta t}{2} T_1\right),$$

$$T_3 = f\left(t_k + \frac{\delta t}{2}, y_k + \frac{\delta t}{2} T_2\right),$$

$$T_4 = f(t_{k+1}, y_k + \delta t T_3)$$

- consistent and convergent of fourth order
- Euler/Heun/Runge-Kutta correspond to rectangle/trapezoidal/Simpson quadrature!



## Alternative: Multistep Methods

- Runge-Kutta-type methods are expensive ☹: many evaluations of  $f$  (sometimes not given in closed form)
- different way to get higher order by profiting from history: Adams-Bashforth-type or multistep methods

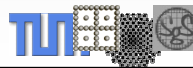
- prominent representative: second-order method

$$y_{k+1} = y_k + \frac{\delta t}{2} (3f(t_k, y_k) - f(t_{k-1}, y_{k-1}))$$

- general form: take polynomial  $P(t)$  interpolating  $f$  in the discrete points of time

$$y_{k+1} = y_k + \int_{t_k}^{t_{k+1}} \dot{y}(t) dt = y_k + \int_{t_k}^{t_{k+1}} f(t, y(t)) dt \doteq y_k + \int_{t_k}^{t_{k+1}} P(t) dt$$

- $p=1$ : Euler;  $p=2$ : above method; generally: order  $p$
- start: no/not enough predecessors available; hence modify!



## Implicit Methods

- All schemes mentioned so far are *explicit* ones: The rule shows a direct way to do another time step.
- now: use the new value  $y_{k+1}$  on the right-hand side, too
- This leads us to Adams-Moulton multistep schemes:

- use interpolation and previous values as with Adams-Bashforth
- second order variant:

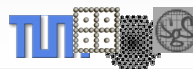
$$y_{k+1} = y_k + \frac{\delta t}{2} (f_k + f_{k+1})$$

- fourth order variant:

$$y_{k+1} = y_k + \frac{\delta t}{24} (f_{k-2} - 5f_{k-1} + 19f_k + 9f_{k+1})$$

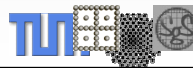
- How to get  $y_{k+1}$  in the implicit case?

- straightforward way: solve the (generally nonlinear) equation
- easier (and widespread): *predictor-corrector* approach



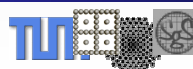
## III-Conditioned Problems

- small changes in input entail completely different results
- Numerical treatment of such problems is difficult!
- an example:
  - consider the ODE  $\ddot{y}(t) - N \cdot \dot{y}(t) - (N+1) \cdot y(t) = 0$
  - initial conditions:  $y(0) = 1, \dot{y}(0) = -1$
  - exact solution:  $y(t) = e^{-t}$
- slight change in initial condition:
  - new value of y in t=0:  $y_\varepsilon(0) = 1 + \varepsilon$
  - resulting new solution:  $y_\varepsilon(t) = \left(1 + \frac{N+1}{N+2} \varepsilon\right) e^{-t} + \frac{\varepsilon}{N+2} e^{(N+1)t}$
  - arbitrarily small change leads to completely different result:  $t \rightarrow \infty$
- risk: non-precise input, round-off errors, ...



## Stability

- consider another IVP:  $\dot{y}(t) = -2y(t) + 1, y(0) = 1$
- exact solution:  $y(t) = (e^{-2t} + 1)/2$
- well-conditioned:  $y_\varepsilon(0) = 1 + \varepsilon \Rightarrow y_\varepsilon(t) - y(t) = \varepsilon e^{-2t}$
- use the midpoint rule:  $y_{k+1} = y_{k-1} + 2\delta t \cdot f_k$   
 $y_{k+1} = y_{k-1} + 2\delta t(-2y_k + 1) = y_{k-1} - 4\delta t \cdot y_k + 2\delta t, y_0 = 1$
- 2-step rule: start with initial value and the exact  $y(\delta t)$ 
  - time step  $\delta t = 1.0 \Rightarrow y_9 = -4945.5, y_{10} = 20953.9$
  - time step  $\delta t = 0.1 \Rightarrow y_{79} = -1725.3, y_{80} = 2105.7$
  - time step  $\delta t = 0.01 \Rightarrow y_{999} = -154.6, y_{1000} = 158.7$
- midpoint rule is second-order consistent, but does not converge here: oscillations or instable behaviour
- there are stability conditions; generally:  
 consistency + stability = convergence



## Stiffness

- for another phenomenon, consider the IVP

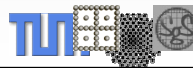
$$\dot{y}(t) = -1000y(t) + 1000, \quad y(0) = y_0 = 2$$

- exact solution:  $y(t) = e^{-1000t} + 1$
- problem well-conditioned
- explicit Euler: stable (as all explicit 1-step methods or all Adams-Bashforth or all s-step Adams-Moulton methods for  $s > 1$  are)
 
$$y_{k+1} = y_k + \delta t(-1000y_k + 1000) = (1 - 1000\delta t)y_k + 1000\delta t$$

$$= (1 - 1000\delta t)^{k+1} + 1$$
- oscillations and divergence for  $\delta t > 0.002$
- Why that? Consistency and stability are *asymptotic* terms. Remedy: Implicit methods (try implicit Euler)!



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## Boundary Value Problems: Outlook

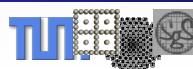
- example:  $\ddot{y} = f(t, y, \dot{y})$ ,  $t_a \leq t \leq t_b$ ,  $y(t_a) = y_a$ ,  $y(t_b) = y_b$
- special case:  $\ddot{y}(t) = a(t)\dot{y}(t) + b(t)y(t) + c(t)$ , same b.c.
- a vanishing and b positive: BVP has unique solution
- discrete grid:  $\delta t = (t_b - t_a) / n$ ,  $t_0 = t_a$ ,  $t_n = t_b$ ,  $t_i = t_a + i\delta t$
- finite difference approximation for second derivative:

$$\ddot{y}(t) \doteq \frac{y(t + \delta t) - 2y(t) + y(t - \delta t)}{\delta t^2}$$

- discrete analogon to ODE in each grid point:
 
$$\delta t^{-2} \cdot (y_{i+1} - 2y_i + y_{i-1}) - b_i y_i = c_i, \quad i = 1, \dots, n-1$$
- tridiagonal system of linear equations
- alternative: shooting methods (reduction to IVPs)



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